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Scaling laws and mechanical properties of nanoporous copper

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ABSTRACT

Through molecular dynamics simulations, the mechanical behavior of nanoporous copper under impact loading was investigated with relative densities ranging from 77.91% to 98.36%, focusing on deformation mechanism, the scaling laws and influence of ligament sizes. Results show that the classical Gibson-Ashby's scaling laws should be modified for prediction of both the Young's modulus and yield stress. A proportional relationship is established between cell wall thickness and yield stress, and new modified scaling equations are built for nanoporous copper with consideration on both relative mass density and size effects of ligaments. The size effect can be explained by larger surface area/volume ratio of samples with thinner ligament size and limited dislocation source activation due to narrow space between larger numbers of voids.

1. Introduction

Nanoporous metals (NPMs) represent an interesting type of nano-structured material with nano-sized porosity and ultrahigh specific surface area, and thus receives significant attention associated with its fabrication and novel properties. Many routes have been reported to prepare nanoporous metals, including free alloy corrosion[1-3], ballistic deposition[4], powder metallurgy[5], electro-deposition[6-8], surfactant emulsion template[9], catalytic chemical deposition method[10], and template-printing method[11], etc.

Nanoporous metals exhibit a uniform, bi-continuous network comprised of nanoscale pores and solid ligaments, and display novel mechanical, chemical, optical and physical properties due to its high surface-to-volume ratio and low densities. The unique characteristics of nanoporous metals can render these unusual properties for advanced applications[12], and NMPs are promising candidates for various fields, such as actuation[13], catalysis[14], tissue engineering and impact-tolerant structures[15,16].

As a fundamental for all applications, mechanical property of NPMs can both strongly affect their structure and performance and lead to failure. Thus, it is important to investigate the mechanical behavior of NPMs under external loadings. Many experimental and theoretical efforts have been devoted to exploring the mechanical behavior of nanoporous Au. Li and Sieradzki[17] observed a microstructural ductile-brittle transition in porous Au which seemed to be controlled by the length scale of the material. Biener et al.[18] studied the plastic deformation of nanoporous Au under compressive stress with depth-sensing nanoindentation and the fracture behavior of the sponge-like materials on the nanometer length scale, which revealed cell-size effects on the microscope failure mechanism of nanoporous metals. Erlebacher et al.[1] and Biener et al.[18,19] also have done tremendous researches to investigate deformation mechanism of nanoporous gold with experimental methods. However, little attention has been devoted to the mechanical behavior of nanoporous copper and other types of metals. Thus, it is inconclusive that these previous results, such as scaling laws, are applicable to any foam metal at nanoscale.

With the majority of reviews dedicated to the experimental and theoretical findings[17,18-21], the computational researches have long been overlooked. In fact, the latter has provided an effective solution in illustrating some physical phenomena which could not be explained by experimental measurement, especially for those controversial issues[13]. Simulated physical phenomena range from fatigue crack propa-

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gation[20], dislocation evolution[21], and shock-induced plasticity[22,23] to softening of nanotwinned metals[24]. Molecular dynamics (MD) is a computer simulation technique, which can describe the movements of atoms or molecules in a large system to obtain their physical properties. The mechanical properties and mechanisms of nanomaterials can be properly investigated with MD simulation techniques. Indeed, it is a useful tool to study the physical and mechanical properties of NPMs which can partly replace the costly experiments.

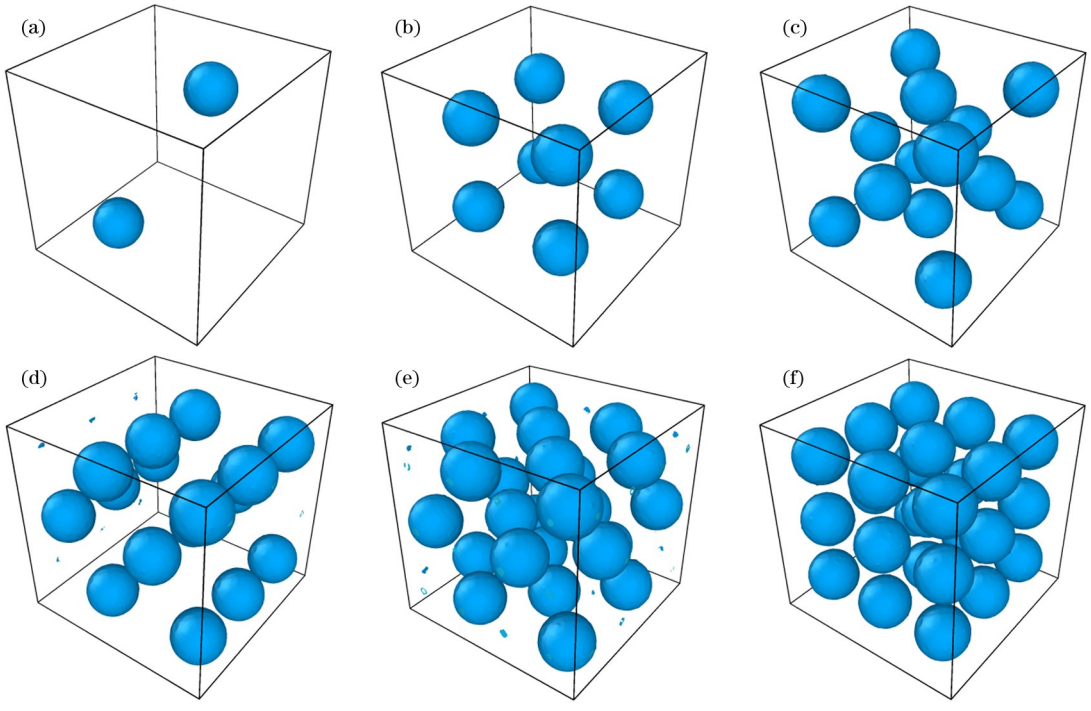
The main focus of this paper is to investigate the mechanical properties of nanoporous copper. A comprehensive study of closed-cell nanoporous copper samples with relative densities ranging from 77.91% to 98.36% was proposed in this study, and the simulation data were compared with the prediction through scaling equations for the Young's modulus and yielding strength in order to capture the link about mechanical properties between nanoporous metals and macropore-sized foams. Furthermore, more efforts have been devoted to investigating the scaling equations for yield stress and effective Young's modulus of nanoporous copper on the basis of the Gibson-Ashby scaling laws and capturing the relationship between deformation behavior and porosities.

2. Simulation Method and Geometrical Models

Molecular dynamics simulations have been shown to be quite useful in studying phenomena on the atomistic scale and can be a potentially powerful tool to investigate the mechanical properties of materials with nanoscale features. Cantrell[25] performed MD simulations at room temperature using Mishin potential on tetrakaidecahedron foam structures to determine whether macro-scale metallic foam theory can be scaled appropriately to nanoporous foams. Atomistic simulations play a two-fold role: not only can they provide unique insights of the process occurring at the nanoscale, but also point out the direction of future study.

MD simulations in this paper were performed through the molecular dynamics code LAMMPS (large-scale atomic/molecular massively parallel simulator) and a Cu embedded atom method (EAM) potential developed by Adams et al.[26]. The validity of these EAM functions has been tested by applying them to a wide variety of bulk and surface properties of both pure metals and binary alloys.

The cubic simulation domain includes a single cubic copper (FCC structure with lattice parameter a_0 = 0.361 nm) containing various numbers of spherical pores of diameter $d = 30a_0 = 10.83$ nm when considering the effect of the relative density, and these pores are distributed without superposition. As shown in Fig. 1, the sample used was of size $120a_0 \times 120a_0 \times 120a_0$. In order to indicate the same features at room temperature, simulations were conducted at an initial temperature of 300 K. The time step for all simulations was set to be 2.0×10^{-15} s. Impact loading was applied to investigate the mechanical properties



(a) 2 pores; (b) 8 pores; (c) 14 pores; (d) 18 pores; (e) 24 pores; (f) 27 pores.

Fig. 1. Schematic atomic structures of relaxed nanoporous copper samples (d = 10.83 nm) with different pores.